Accuracy of bosonization for localized interactions

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Bosonization is commonly used to calculate the ground-state energy and the dynamics of simple model nonmagnetic impurities in metals. We analyze the accuracy of this procedure in the calculation of the ground-state energy of a simple, solvable, model.

It is generally agreed that bosonization is a useful scheme for understanding the static and dynamic properties of nontrivial one-dimensional many-body systems, whether the interacting entities are fermions or spins. It is acknowledged to be an accurate scheme for the study of low-energy dynamical phenomena, especially those phenomena restricted to the neighborhood of the Fermi surface. But is it trustworthy in the calculation of ground-state energy and excited-state properties when we are dealing with highly localized interactions? This is not a purely academic question, for it impacts on the phase diagram of dilute intermetallic alloys and on related issues. In this paper, we estimate the accuracy of bosonization for the calculation of the ground-state energy using a model of a single impurity site embedded in a gas of otherwise noninteracting fermions. Our results may help set error bounds in other applications, wherever there is a hope that bosonization might yield qualitatively correct results.

For our example, we considered a simple metal consisting of a half-occupied *s*-type conduction band of noninteracting electrons. Now, the atom at the origin is replaced by an impurity atom which is assumed to differ from the host only slightly, and only locally. Its effects can then be modeled by one- or two-body interactions localized at the origin, as in the following Hamiltonian:

$$H=\sum_{k,\sigma}\varepsilon(k)c^{+}_{k,\sigma}c_{k,\sigma}+V(n_{\uparrow}+n_{\downarrow})+Un_{\uparrow}n_{\downarrow},\quad \text{with}$$

$$n_{\sigma}=\frac{1}{N}\sum_{k,k'}c^{+}_{k,\sigma}c_{k',\sigma}, \tag{1}$$

where σ indicates the electrons' spin orientations. In this form it is the well-known Wolff model-impurity.[1] Starting with Wolff's own Hartree-Fock solution[1] this type problem has been analyzed by many authors with the aid of any number of increasingly sophisticated many-body techniques. Here, we consider ''bosonization,'' and/or its converse, ''refermionization,'' in the parameter range such that no bound states lie below the continuuum.

While it is not surprising that the correspondence between low-lying fermionic dynamics and its bosonic representation fails at large values of U (or V) it is reasonable to expect this procedure to become exact in weak coupling. There are many aspects of magnetic and nonmagnetic impurities in nonmagnetic metals of current interest[2] for which a Hamiltonian of type (1) centered at one or several points on the lattice is a good starting point. By comparing results obtained in different ways, we find that exact results are guaranteed *only* in the first order of perturbation theory. Second-order corrections can be correct, or can be off by a factor of 2 or more, while higher-order terms are *always* wrong. We have restricted the parameters to positive values so that bound states, if any, lie above the continuum and therefore do not affect the ground-state calculation.

What follows is a cautionary tale of whether bosonization and its inverse may be applied to the calculation of ground-state energies. Ultimately, the source of the quantitative errors come down to the existence of a finite energy bandwidth, the magnitude of ratios of various quantities to that bandwidth, and to the various scales of energy. In terms of RG theory the one-body terms in Eq. (1) have scaling dimension 1 and are (marginally) relevant while localized two-body interactions have scaling dimension 2 and are not.

To bosonize, it is useful to linearize about the Fermi energy, i.e., set $\varepsilon(k)=\nu_F(k-k_F)$, with (in some appropriate units) $\nu_F=(2\pi)^{-1}$ and $k_F=\pi$. Linear combinations of Bloch states labeled by k in the range $0<k<2\pi$, and zero angular momentum,[3] radiate spherically from the origin. Only *s* waves can interact with the impurity at the origin. We express this interaction in one of two ways. The first is with fermion operators c,

$$H_0=\frac{1}{2\pi}\sum_{k}(k-\pi)c^{+}_{k,\sigma}c_{k,\sigma},\quad \text{as in Eq. (1), while the}$$

$$\text{second uses } H_0=\frac{1}{2\pi}\sum_{q>0}^{Q}\sum_{\sigma}qb^{+}_{q,\sigma}b_{q,\sigma}, \tag{2}$$

in which the b's refer to bosonic operators[4] and $Q=\pi\sqrt{2}$ is the cutoff. These operators are

$$b^{+}_{q,\sigma}=\sqrt{\frac{2\pi}{qN}}\sum_{k}c^{+}_{k+q\sigma}c_{k\sigma},$$

$$b_{q,\sigma}=\sqrt{\frac{2\pi}{qN}}\sum_{k}c^{+}_{k,\sigma}c_{k+q,\sigma},\quad q>0. \tag{3}$$

The usual commutation relations are satisfied,

$$[b_{q,\sigma},b^{+}_{q',\sigma'}]=\delta_{q,q'}\delta_{\sigma,\sigma'}. \tag{4}$$

This result is deceptively simple. For if, instead of Eq. (3), we had required a different linear combination—say, $\tilde{b}_{q,\sigma}=\sqrt{2\pi/qN}\Sigma_k A_{k,q}c^{+}_{k,\sigma}c_{k+q,\sigma}$ with nontrivial amplitudes

$A_{k,q}$—the commutation relations (4) could not be satisfied and the algebra would not close. Just as was the case for H_0, the total Hamiltonian H including interactions can be expressed as a quadratic form in the bosons and be replaced by

$$H=\frac{1}{2\pi}\sum_{q>0,\sigma} qb^{+}_{q,\sigma}b_{q,\sigma}+V\left\{1+\sum_{q>0}\sum_{\sigma}\sqrt{\frac{q}{2\pi N}}(b^{+}_{q,\sigma}+b_{q,\sigma})\right\}+U\left\{\frac{1}{2}+\sum_{q>0}\sqrt{\frac{q}{2\pi N}}(b^{+}_{q,\uparrow}+b_{q,\uparrow})\right\}\times\left\{\frac{1}{2}+\sum_{q>0}\sqrt{\frac{q}{2\pi N}}(b^{+}_{q,\downarrow}+b_{q,\downarrow})\right\}. \tag{5}$$

The constants are eigenvalues of the average occupancies, $\langle N_\sigma\rangle/N=1/N\Sigma_k c^{+}_{k,\sigma}c_{k,\sigma}=\frac{1}{2}$, for a half-filled band. Although they are nominally operators, macroscopic quantities such as the $\langle N_\sigma\rangle/N$'s cannot be affected to $O(1)$ by the presence of a single impurity nor, for that matter, by any finite number of impurities.[5] All q sums are cut off at Q. Here, we have used a representation adapted to the half-filled band for the occupation operators at the impurity site

$$n_\sigma=\frac{1}{2}+\sum_{q>0}^{Q}\sqrt{\frac{q}{2\pi N}}(b_{q,\sigma}+b^{+}_{q,\sigma})=\frac{1}{2}+\delta n_\sigma. \tag{6}$$

The fermionic identity $n_\sigma^2=n_\sigma$, which is trivially satisfied by the operators in Eq. (1) is only satisfied in the bosonic representation if one sets the cutoff at $Q=\pi\sqrt{2}$ and ignores, or projects out, all 2-boson states labeled by equal σ in the calculation of n_σ^2. If same-spin bosons are created in large numbers by the interactions, bosonization will necessarily fail to faithfully represent the original dynamics. Our calculation seeks to estimate by how much it does so.

The bosonization transformation consists of expressing Eq. (1) in the form (5). Its inverse (*re*-fermionization) replaces Eq. (5) by some new underlying fermions (e.g., *spinons* and *holons*.) To illustrate, we shall distinguish two cases, and compute the energy shift $\Delta E_0(V,U)$ in each. In the first case following, we set the two-body potential parameter $U=0$ and retain only the one-body potential V. The Hamiltonian in Eq. (1) can then be diagonalized exactly.

At small V the perturbation-theoretic expansion converges, yielding a Taylor series: $\Delta E_0(V,0)=V-aV^2+bV^3+\cdots$. Then the exact energy shift calculated from Eq. (1) is

$$\Delta E_0(V,0)=V+2\int_0^V dg\int_{-1/2}^{0}d\varepsilon\,\rho(\varepsilon)[\,|1-gS(\varepsilon)|^{-2}-1\,], \tag{7}$$

in which $S(\varepsilon)=\int_{-1/2}^{+1/2}d\varepsilon'\,\rho(\varepsilon')(\varepsilon-\varepsilon')^{-1}=R(\varepsilon)+i\pi$, using a density of states $\rho(\varepsilon)=1$ appropriate to the assumption $\nu=\partial\varepsilon/\partial k=\nu_F=$constant. A bound state that forms above the continuum affects neither the ground state nor its power series expansion. The factor 2 in front of the integral comes from Kramers' (spin) degeneracy. After some simple algebra we get the leading coefficient: $a_{\rm exact}=(\frac{3}{4}-\frac{1}{2}\log 2)=0.600...$.

The corresponding calculation involving Eq. (5) starts by noting that for $U=0$ the nontrivial operator involves the b's only in the form $b_{q,\uparrow}+b_{q,\downarrow}=\sqrt{2}b_{q,+}$, i.e., it only concerns the charge-fluctuation channel. Corresponding spin density fluctuations $b_{q,\uparrow}-b_{q,\downarrow}=\sqrt{2}b_{q,-}$ are absent from the Hamiltonian. Thus the Hamiltonians in the $(+)$ and $(-)$ sectors decouple and can be separately refermionized.

We rewrite the $H_\pm$ in terms of their individual underlying spinons s_k and holons c_k. As there is no interaction term in the former, it suffers no energy shift and its states remain those of free, unscattered particles. The latter acquires interactions of the form

$$H_+=\sum_k \varepsilon(k)c_k^{+}c_k+V[\,1+(n-1/2)\sqrt{2}\,] \tag{8}$$

obtained by using the identity (6), $\delta n_+=n-1/2$. The form of Eq. (8) is independent of the cutoff Q—i.e., there is no ''fudge factor'' in this approach. Except for trivial details (8) is of the same form as Eq. (1) at $U=0$, and thus it similarly yields

$$\Delta E_{0,\rm holon}(V,0)=V+\int_0^{V\sqrt{2}}dg\int_{-1/2}^{0}d\varepsilon\,\rho(\varepsilon)\times[\,|1-gS(\varepsilon)|^{-2}-1\,] \tag{9}$$

again with $\rho(\varepsilon)=1$. The bandwidth, the one-particle density of states and the Fermi velocity are the same in Eq. (8) as in Eq. (1). Although there is no Kramers' factor 2 the effective interaction for holons is greater by a factor $\sqrt{2}$ than for the original electrons. The result is that $a=a_{\rm exact}$. In this example, bosonization followed by its inverse yields an answer which is exact to $O(V^2)$. The errors inherent in the two procedures have canceled exactly. But before celebrating one should note that this cancellation of errors does not persist in higher orders. Already the coefficient b of the cubic term as extracted from Eq. (9) is wrong. Indeed, by comparison of the exact Eq. (7) to the approximate result in Eq. (9) one sees that for all $n>2$ the coefficient of V^n in the latter exceeds the former, by a factor $2^{(n/2-1)}$.

Had we *not* refermionized the results would be cut-off dependent, and numerically not as good. For when we use the boson Hamiltonian Eq. (5) directly to compute the coefficient a, we obtain a number some 2.3 times larger than the exact value. As for the higher-order coefficients in $n^{\rm th}$ order of the perturbation expansion of Eq. (5), for $n>2$ they all are wrong, as they vanish regardless of the choice of Q.

The two approximations are compared with each other and with the exact result in Fig. 1. We plot $\Delta E-V$ to emphasize the differences. The refermionized ΔE is quite close to the exact value in the weak-coupling range which, for numerical purposes, we take to be $0<V<0.6$, while (exact) second order perturbation theory is reasonably accurate only for $0<V<0.4$. By contrast, the boson Hamiltonian with the canonical cutoff Q is accurate nowhere, unless the cutoff were to be arbitrarily reduced by a substantial factor, one which cannot be determined *a priori* without knowledge of the exact answer.

We next examine the 2-body force. One-body terms are canceled by setting $V=-U/2$. In this example, the agreement between the original model and its bosonized versions fail already in the second order of U (the ''irrelevant,'' nonuniversal interaction, in the language of RG.) We shall compare the coefficients α in the expansion,

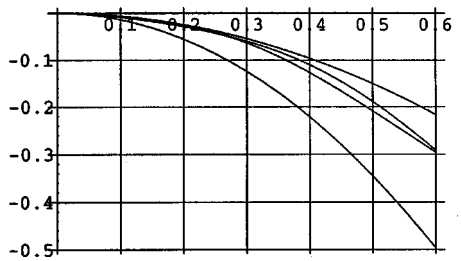

FIG. 1. Plot of $\Delta E(V,0)-V$, as function of V, in weak-coupling, in units of the conduction bandwidth. The top curve is parabolic, and is the result of the second-order perturbation theory (calculated exactly). The next curve from the top is the exact result, to all orders, extracted from Eq. (7). The second curve from the bottom is obtained using the ''refermionization'' procedure, as given in Eq. (9), and has no adjustable parameters. It is seen to be in fairly good agreement with the exact curve—especially in the range $0<V<0.25$ and again at 0.6, although not at larger V. The lowest curve results from the bosonized approximation in Eq. (5) and it is cutoff dependent. Here, we use the correct cutoff $Q=\pi\sqrt{2}$, as discussed in Eq. (6) *ff*. Using hindsight, and arbitrarily reducing the cutoff to agree with the exact results at $V=0$, one *could* shift this curve into coincidence with the top curve. Even so, the latter deviates visibly from the exact result for all $V>0.4$.

$$\Delta E_0\left(-\frac{U}{2},U\right)=-U/4-\alpha U^2+\beta U^3+\cdots, \tag{10}$$

calculating the ''exact'' α from Eq. (1). Taking advantage of the symmetry at half-filling we obtain from ordinary perturbation theory the expression

$$\alpha_{\text{exact}}=\int_0^{1/2}d\varepsilon_1\int_0^{1/2}d\varepsilon_2\int_0^{1/2}d\varepsilon_3\int_0^{1/2}d\varepsilon_4(\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4)^{-1}=0.070\ldots. \tag{11}$$

Note that this coefficient is almost one order of magnitude smaller than the corresponding coefficient a of the one-body potential. The bosonic Hamiltonian (5) yields a Q-dependent value

$$\alpha_{\text{boson}}=\left(\frac{Q}{\pi}\right)^3\int_0^{1/2}d\varepsilon_1\varepsilon_1\int_0^{1/2}d\varepsilon_2\varepsilon_2(\varepsilon_1+\varepsilon_2)^{-1}=0.4546(Q/2\pi)^3. \tag{12}$$

Using $Q=\pi\sqrt{2}$ we obtain a coefficient α that, once again (and perhaps coincidentally,) is just 2.3 times larger than the correct value, as given in Eq. (11).

Even more notably refermionization, which gave good agreement in the preceding example, fails here. We start with Eq. (1) in the form

$$H=H_0-U/4+U\,\delta n_\uparrow\,\delta n_\downarrow, \tag{13a}$$

which we can rewrite as

$$H=H_0-U/4+U(\delta n_+^2-\delta n_-^2)/4=H_0-U/4+U\{(n_+-1/2)^2-(n_--1/2)^2\}/4. \tag{13b}$$

We now invoke the identity in Eq. (6): $(n_\pm-1/2)^2=1/4$. The terms in the curly brackets cancel one another, therefore $\alpha=0$ in this representation; all higher order coefficients in the expansion (10) vanish also. Is this a serious error? Given the smallness of α in Eq. (11), perhaps this brings in no significant error in the range $0<U<1$, although the suppression of quantum fluctuations is troubling.

Recapitulating: we have investigated the accuracy of bosonization in the calculation of the ground-state energy of an exactly solvable model impurity in a free-electron metal, and find it to be entirely satisfactory only in the weak-coupling regime. We have not addressed the low-energy dynamics for which the matrix elements and level spacings may (or may not!) be rendered more faithfully by bosonization than was the ground state. Nor have we investigated attractive potentials, for which bound states below the continuum contribute to the ground state energy, making the comparisons more difficult. These topics should be examined separately.

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[1] P. A. Wolff, Phys. Rev. **124**, 1030 (1961). If V and U exist at every site, the model transmutes into the Hubbard model, with very much different properties. In particular, V becomes absorbed into the chemical potential and is no longer relevant, while U acquires scaling dimension 1 and now becomes relevant.

[2] Including the Kondo effect and its competition with long-range oscillatory interactions—see I. Affleck, A. W. W. Ludwig, and B. A. Jones, Phys. Rev. B **52**, 9528 (1995) and earlier references therein.

[3] More accurately, having the point-group symmetry of the crystal.

[4] D. C. Mattis and E. H. Lieb, J. Math. Phys. **6**, 304 (1965).

[5] Changes $O(1/N)$ are allowed but are inconsequential.